

# $\pi$ -junction to probe antiphase s-wave pairing in iron pnictide superconductors

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(Dated: November 12, 2009)

Josephson junctions between a *FeAs*-based superconductor with antiphase s-wave pairing and a conventional s-wave superconductor are studied. The translational invariance in a planar junction between a single crystal pnictide and an aluminum metal greatly enhances the relative weight of electron pockets in the pnictide to the critical current. In a wide doping region of the pnictide, a planar and a point contact junctions have opposite phases, which can be used to design a tri-junction ring with  $\pi$  phase to probe the antiphase pairing.

PACS numbers: 74.70.Dd, 71.30.+h, 74.20.Mn

One of important issues for the newly discovered iron pnictide superconductors (SCs) [1, 2, 3, 4, 5, 6, 7, 8, 9] is their pairing symmetries. A number of experiments [10, 11, 12, 13] have suggested a spin singlet s-wave pairing. The iron pnictide has hole and electron Fermi pockets (Fig. 1). Theories have predicted an antiphase s-wave or  $s_{\pm}$  state, where the pairing has an s-wave symmetry, but the order parameters on the electron and hole pockets have opposite signs [14, 15, 16, 17, 18, 19]. It will be important to confirm the  $s_{\pm}$  state for pnictides, especially using more decisive phase sensitive experiments, which provided a direct evidence for the  $d_{x^2-y^2}$  pairing for cuprates[20, 21]. Since  $s_{\pm}$  phase is related to the  $\vec{k}$ -space location instead of the orientation, different types of phase sensitive experiments are needed to probe the signs of the gap functions[22, 23, 24, 25, 26]. Very recently, Chen et al.[13] have carried out a new phase sensitive experiment on polycrystal *NdFeAsO* compound, and observed integer and half integer flux quantum transitions in a niobium/Fe-pnictide loop, which clearly demonstrates the sign changes of the order parameters in Fe-pnictides.

In this Letter, we study Josephson junctions between a *FeAs*-based SC of  $s_{\pm}$ -pairing and a conventional s-wave SC. The translational invariance in a planar junction between a single crystal pnictide and an aluminum metal greatly enhances relative weight of electron pockets to the critical current. In a wide doping region for both *BaFe<sub>2</sub>As<sub>2</sub>* (122 hereafter) and *LaFeAsO* (1111 hereafter) compounds, a planar and a point contact junctions have opposite phases. This property can be used to design a tri-junction ring with  $\pi$  phase to probe the antiphase s-wave pairing.

We start with a brief review on the charge current  $I_J$  passing through a Josephson junction of two conventional SCs.  $I_J = I_c \sin \delta\phi$ , with  $I_c$  the critical current, and  $\delta\phi$

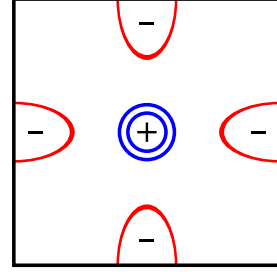


FIG. 1: Schematic plot of Fermi surface of pnictide in an extended Brillouin zone where each unit cell contains one Fe-ion. Signs represent phase of the superconducting gap.

the phase difference between the two SCs. In the absence of magnetic fields or magnetic impurities, we may focus on  $I_c$ , which is of the form

$$I_c \propto \int d\mathbf{k} d\mathbf{q} \frac{|T_{\mathbf{k}\mathbf{q}}|^2 \Delta_1(\mathbf{k}) \Delta_2(\mathbf{q})}{E_1(\mathbf{k}) E_2(\mathbf{q}) [E_1(\mathbf{k}) + E_2(\mathbf{q})]}, \quad (1)$$

where  $T_{\mathbf{k}\mathbf{q}}$  is the tunneling matrix,  $E_i(\mathbf{k}) = \sqrt{\epsilon_i(\mathbf{k})^2 + \Delta_i(\mathbf{k})^2}$  is the quasiparticle energy of the SC  $i = 1, 2$ ,  $\epsilon_i(\mathbf{k})$  is the single electron energy measured relative to the chemical potential, and  $\Delta_{1(2)}$  are superconducting gap functions (assumed to be real). The proportional coefficient in  $I_c$  are always positive throughout this paper. The junction is a 0-junction if  $I_c > 0$ , and a  $\pi$ -junction if  $I_c < 0$ . If both SCs are simple s-wave,  $\Delta_i(\mathbf{k})$  are independent of  $\mathbf{k}$ , and the sign of  $I_c$  is determined by the relative signs of  $\Delta_1$  and  $\Delta_2$ . Though  $\Delta$  is not gauge invariant, Sigrist and Rice[27] have pointed out that the  $\pi$ -junctions can not be gauged away if there are odd numbers of  $\pi$ -junctions in a loop.

Eq. (1) can be extended to study Josephson junctions between a pnictide and a conventional SC. Let  $\Delta_2$  be the superconducting gap and  $E_2(\mathbf{q})$  the quasi-particle energy

of a conventional s-wave SC, and  $\gamma$  the band index of the pnictide. We shall neglect the inter-band pairing amplitude in the pnictide, whose effect is small due to the energy splitting of the bands [19]. Denoting  $\Delta_1^\gamma(\mathbf{k})$  the superconducting gap of the band  $\gamma$  and  $E_1^\gamma(\mathbf{k})$  the corresponding quasi-particle energy, we have

$$I_c \propto \Delta_2 \sum_\gamma \int d\mathbf{k} d\mathbf{q} \frac{|T_{\mathbf{k}\mathbf{q}}|^2 \Delta_1^\gamma(\mathbf{k})}{E_1^\gamma(\mathbf{k}) E_2(\mathbf{q}) [E_1^\gamma(\mathbf{k}) + E_2(\mathbf{q})]}. \quad (2)$$

Because of small value in  $\Delta/E$  for states far from the Fermi surface, the integral in Eq. (2) is of appreciable value only for  $\mathbf{k}$  and  $\mathbf{q}$  near their Fermi surfaces. The Fermi pockets in Fe-pnictide are well separated, so we may replace  $\sum_\gamma \int d\mathbf{k}$  in Eq. (2) by integrals over  $\mathbf{k}$  within a small cut-off around each Fermi pocket  $\alpha$ . Assuming  $\Delta_1^\alpha$  to be isotropic near each Fermi pocket  $\alpha$ , we have

$$I_c \propto \Delta_2 \sum_\alpha \Delta_1^\alpha \int d\mathbf{k} d\mathbf{q} \frac{|T_{\mathbf{k}\mathbf{q}}|^2}{E_1^\alpha(\mathbf{k}) E_2(\mathbf{q}) [E_1^\alpha(\mathbf{k}) + E_2(\mathbf{q})]}, \quad (3)$$

where the sum of  $\alpha$  is over all the Fermi pockets within the Brillouin zone (BZ), and integral of  $\mathbf{k}$  is over around the Fermi pocket  $\alpha$  within a small cut-off.

We choose a convenient gauge where the gap function of the conventional s-wave SC is positive and the gap function of the hole (electron) pockets in the Fe-pnictide SC is positive (negative). To simplify the calculations, we shall neglect the dispersion of the Fermi surface in the direction perpendicular to the Fe-plane in the pnictide [11]. In what follows we will use Eq. (3) to study point and planar junctions. While our formalisms may be applied to all the iron-based SC, we will primarily discuss 122-based SC for its availability of good single crystals. The junctions for 1111-based SC will be briefly discussed.

*Point junction between  $s_\pm$  and s-wave SC.* For point junction, there is no momentum conservation in the tunneling. The tunneling direction relative to the FeAs plane is also random, so that the tunneling matrix is insensitive to the d-orbitals hence to the bands in the Fermi pockets. We may then set  $T_{\mathbf{k}\mathbf{q}} = T_0$  to be a constant, and Eq. (3) becomes

$$I_c \propto |T_0|^2 \sum_\alpha \Delta_1^\alpha \Delta_2 N_{1F}^\alpha N_{2F} \int d\epsilon_1 d\epsilon_2 \frac{1}{E_1^\alpha E_2 [E_1^\alpha + E_2]},$$

where  $N_{1F}^\alpha$  and  $N_{2F}$  are the density of states (DOS) on the Fermi pocket  $\alpha$  of the pnictide and of the s-wave SC at the Fermi level, respectively. Following Ambegaokar and Baratoff [29], assuming  $\Delta_2 \ll |\Delta_1^\alpha|$ , we have

$$I_c \propto N_{2F} \Delta_2 \sum_\alpha \text{sgn}(\Delta_1^\alpha) N_{1F}^\alpha K \left[ \sqrt{1 - \frac{\Delta_2^2}{(\Delta_1^\alpha)^2}} \right], \quad (4)$$

where  $K(x)$  is the first kind complete elliptic integral. The amplitude of  $\Delta_1^\alpha$  of the Fe-pnictide are of the same order [11]. In the limit of  $|4\Delta_1^\alpha/\Delta_2| \gg 1$ ,  $I_c$  is given by

$$I_c \propto \sum_{\alpha \in BZ} \text{sgn}(\Delta_1^\alpha) N_{1F}^\alpha. \quad (5)$$

where the sum is over pockets  $\alpha$  within the BZ. Therefore,  $I_c > 0$  if the hole DOS  $N_h$  is larger than the electron DOS  $N_e$ , and  $I_c < 0$  if  $N_h < N_e$ . We have carried out density functional theory (DFT) calculations and the results for 122-compounds are shown in Fig. 2(a). From the figure, the point contact junctions are 0-junctions except at very large electron doping.

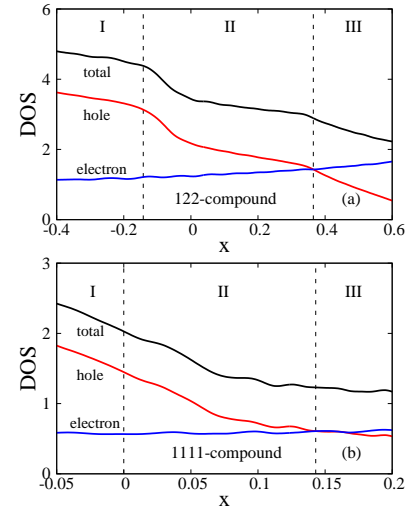


FIG. 2: (color online) Hole DOS  $N_h$  (red curve) and electron DOS  $N_e$  (blue curve), and total DOS vs doping  $x$  for 122-compound (a) and 1111-compound (b), where  $x > 0$  for electron and  $x < 0$  for hole dopings. The point junction is a 0-junction in Region I and II, and a  $\pi$ -junction in Region III. The planar junction is a 0-junction in Region I, and a  $\pi$ -junction in Region II and III. So the tri-junction loop in Fig. 4 has a  $\pi$ -phase in Region II.

*Planar junction.* We now consider a junction between a 122 single crystal and a nearly free electron Al with a spherical Fermi surface, as shown in Fig. 3. The thin insulator plane in the junction is parallel to the FeAs-plane ( $x-y$  plane) of the pnictide. In a nearly free electron metal, the lattice potential of the material is very weak, so that we may neglect the lattice effect, and the junction has a translational symmetry in the  $x-y$  plane. Otherwise, we assume the tunneling matrix element to be independent of the Fermi pockets,  $T_{\mathbf{k}\mathbf{q}} = T_0 \delta_{k_{xy}, q_{xy}}$ , where  $k_{xy}$  and  $q_{xy}$  are the planar wavevectors. This assumption is valid if there are only two orbitals  $d_{xz}$  and  $d_{yz}$  are involved, for they are related by a  $90^\circ$  rotational symmetry. In Fe-pnictide, there are five  $d$ -orbitals with more weight on  $d_{xz}$  and  $d_{yz}$ , but finite weight on others [30]. We expect that our approximation be reasonably

good, and will return to discuss the correction to this approximation.

It is convenient to work on the repeated zone scheme, where the BZ of the wavevector  $\mathbf{k}$  of the pnictide is expanded into an infinite plane. Because of the planar momentum conservation, noting that the integral in Eq. (2) is only of appreciable value near the Fermi surfaces/pockets, Eq. (3) becomes,

$$I_c \propto |T_0|^2 \Delta_2 \int_{|k_{xy}| < q_F} dk_{xy} dq_z \sum_{\alpha} \frac{\Delta_1^{\alpha}}{E_1^{\alpha}(k_{xy}) E_2(k_{xy}, q_z)} \times \frac{1}{E_1^{\alpha}(k_{xy}) + E_2(k_{xy}, q_z)} \quad (6)$$

where  $q_F$  is the Fermi wavevector and  $q_z$  the z-component wavevector of the conventional SC. The sum of  $k_{xy}$  is within the circle of a radius  $q_F$  in the x-y plane, and  $\sum_{\alpha}$  stands for the summation over all the Fermi pockets within the circle of radius  $q_F$  as illustrated in Fig. 3. The tunneling process for the wavevector outside the BZ is due to the umklapp process.

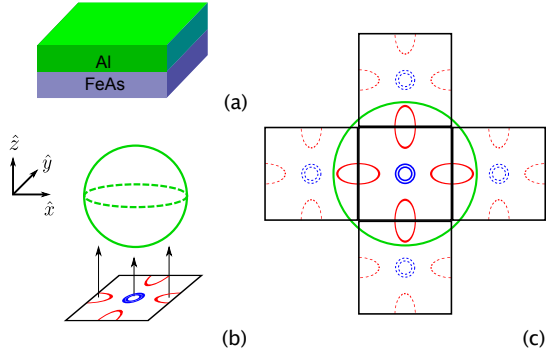


FIG. 3: (color on line) (a) Proposed planar junction, whose interface is parallel to the  $x-y$ -plane. (b) Illustration of electron tunneling (black arrows) with planar momentum conservation. Top sphere (green): Fermi surface of Al metal; bottom: Fermi surface of Fe-pnictide. (c) Fermi surface of Al (green line) and Fe-pnictide (blue lines for hole and red for electron pockets) at  $q_z = 0$ . Black lines are the BZ boundary. The Fermi pockets outside the green circle has no contribution to the Josephson current.

For a free electron metal, we have  $\int dq_z \approx \frac{C}{\sqrt{q_F^2 - k_{xy}^2}} \int d\epsilon_2$ , with  $C$  a constant. To further calculate  $I_c$ , we approximate  $k_{xy}$  in the term of  $1/\sqrt{q_F^2 - k_{xy}^2}$  by a mean squared average of the wavevector  $Q_{\alpha}$  within the Fermi pocket  $\alpha$ , and obtain

$$I_c \propto T_0^2 \Delta_2 \sum_{\alpha \in q_F} \frac{\text{sgn}(\Delta_1^{\alpha}) N_{1F}^{\alpha}}{\sqrt{q_F^2 - Q_{\alpha}^2}} K\left(\sqrt{1 - \frac{\Delta_2^2}{(\Delta_1^{\alpha})^2}}\right) \sim \Delta_2 \sum_{\alpha} \frac{\text{sgn}(\Delta_1^{\alpha}) N_{1F}^{\alpha}}{\sqrt{q_F^2 - Q_{\alpha}^2}} \quad (7)$$

For Al, the Fermi surface is a sphere (see Fig. 3(b)) of a radius of the Fermi wavevector  $q_F = 1.75 \text{\AA}^{-1} = 1.56\pi/a$ , with  $a = 2.8 \text{\AA}$  the distance of two nearest neighbor irons in 122 compound. As we can see from Fig. 3(c), the area hence the DOS of the electron pockets enclosed within a circle of  $q_F$  is twice of the area or the DOS within the BZ of the Fe-pnictide. By using Eq. (7) and the results of  $N_e$  and  $N_h$  from DFT, approximating  $Q_{\alpha} = \pi/a$  for the electron pockets, and  $Q_{\alpha} = k_F^h(k_z = 0)$ , the Fermi momentum for the hole pockets, we find  $I_c < 0$  when  $N_h/N_e < 2.58$  which corresponds to the region II and III in Fig. 2(a). In our calculations, we have assumed the tunneling matrix to be independent of the momentum or the Fermi-pockets. In 122 compounds, in addition to  $d_{xz}$  and  $d_{yz}$  orbitals, the electron configuration on the hole pockets contains  $d_{3z^2-1}$  orbital, and also contains more  $d_{x^2-y^2}$  or  $d_{xy}$  orbitals than on the electron pockets. Because of their orbital orientations, the  $d_{3z^2-1}$  orbital enhances the tunneling matrix, and the  $d_{x^2-y^2}$  and  $d_{xy}$  orbitals do the opposite. Therefore, their overall effect to the condition of the  $\pi$ -junction is partially canceled. We expect the results obtained by this approximation to be qualitative or semi-qualitatively correct.

We have also combined DFT results and ARPES data to calculate  $I_c$  and obtained similar results. In the calculation, we use Eq. (3) directly by taking into account of the planar momentum conservation. We apply a rigid band approximation for the normal state electron state in DFT and take the gap functions of the hole doped 122 compound from ARPES data of Ding et al. The dispersion in Al is modeled by  $\epsilon_{\mathbf{q}} = q^2 \hbar^2 / 2m^*$ , with the effective mass of the electron  $m^* = 1.16m_e$ , and  $m_e$  the free electron mass. We assume a BCS gap function for Al SC at  $T=0$  based on value of  $T_c = 1.175K$ . We have found the planar junction is of  $\pi$ -phase at hole doping up to 0.4, which gives a wider region for the  $\pi$ -junction.

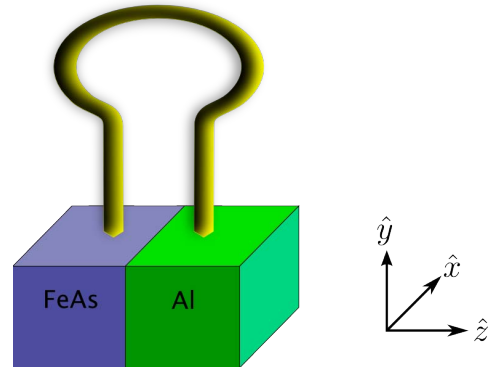


FIG. 4: A Tri-junction setup, consisting of a planar junction between Al and Fe-pnictide SC, and a point junction between a conventional SC (say niobium) and Al and a point junction between the niobium and the pnictide.

*Tri-junction to probe  $s_{\pm}$  symmetry* We now discuss Josephson tri-junction to probe the  $s_{\pm}$ -pairing in Fe-

pnictide SC. The experimental setup is illustrated in Fig. 4, similar to that in Ref. [13]. Fe-pnictide is chosen so that its planar junction with Al is a  $\pi$ -junction, and its point junction with niobium is a 0-junction. The tri-junction configuration is then a  $\pi$ -loop characterized by half-integer flux quantization. The condition for the such a  $\pi$ -junction of the planar and 0-junction of the point junctions is illustrated in Fig. 2(a) for 122-compound. As we can see, there is a large region of the material space to satisfy the  $\pi$  tri-junction condition.

Let us briefly discuss the electron doped 1111-compound, which will be important when its single crystal becomes available. Our DFT calculations show that  $N_h/N_e > 1$  at the doping  $x < 0.15$ , and  $N_h/N_e < 1$  at  $x > 0.15$ . Therefore, its point junction with a conventional SC will be a 0-junction at  $x < 0.15$  and a  $\pi$ -junction at  $x > 0.15$ , as shown in Fig. 2(b). A planar junction between 1111-compound and Al SC is found to have  $\pi$ -phase for all the electron doped region studied. Hence a set-up in Fig. 4 for 1111 with  $x < 0.15$  is expected to be a  $\pi$  junction loop.

We remark the implication of the experiment observation of the  $\pi$ -junction loop in the set-up of Fig. 4. A  $\pi$ -junction indicates the opposite phases in the point and planar junctions the FeAs SC is involved. This would rule out a conventional s-wave pairing, or a d-wave pairing such as  $d_{x^2-y^2}$  or  $d_{xy}$ . The later will result in a vanishing critical current in a junction with a s-wave SC. Thus the observation of the  $\pi$ -junction loop should be a clear indication of the  $s_{\pm}$  pairing state for the FeAs SC.

*Tri-junction with two-pnictide SCs* We now turn to a discussion of a Josephson tri-junction ring, consisting of two single crystal Fe-pnictides and one conventional SC, say niobium. The junctions between each of the Fe-pnictide and the niobium are both point contact, and the junction between the two pnictides is a planar one with the junction plane parallel to the FeAs planes in both the pnictides. We request  $N_h > N_e$  in the first Fe-pnictide, and  $N_h < N_e$  in the second Fe-pnictide. Therefore, one of the point junctions is 0-junction, and the other is  $\pi$ -junction. The pnictide-pnictide planar junction is a 0-junction because of the  $x-y$  plane crystal momentum conservation in the tunneling process, where the tunnelings only occur between hole pockets or between electron pockets in the two SCs. The tri-junction ring thus designed should have a  $\pi$ -junction in nature. The experimental challenge to design this tri-junction is related to the sample quality and the selection of the second Fe-pnictide where the electron DOS is larger. The DFT calculations suggest that 1111-compound is a good candidate for this type of tri-junctions when the single crystals become available.

In summary, we have examined the phase of the Josephson junctions between Fe-pnictide and conventional s-wave superconductors. The sign of a point-contact junction is positive if the hole DOS is larger than

the electron DOS in Fe-pnictide and is negative otherwise. In the planar junction between a single crystal Fe-pnictide and Al, planar translational invariance in the tunneling enhances the contribution of electron pockets to the critical current. We have proposed a Josephson tri-junction to probe the  $s_{\pm}$  symmetry in Fe-pnictide, which appears to be accessible in experiments.

We thank C. C. Tsuei, T. M. Rice, and C. C. Chi for many useful discussions. This work is supported in part by HKSAR RGC grant and by NSFC and by National Program for Basic Research of MOST, China, and by KITPC through the Project of Knowledge Innovation Program (PKIP) of CAS, Grant No. KJCX2.YW.W10.

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